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**A COMPUTATIONAL EFFICIENT PHYSICS BASED
METHODOLOGY FOR MODELING CERAMIC MATRIX
COMPOSITES (PREPRINT)**

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Materials Sciences Corp.

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ABSTRACT

The purpose of this study is to demonstrate the feasibility of modeling inelastic responses of ceramic matrix composites (CMC), where deviations from elastic behavior are primarily due to micro-crack evolution within the material. The theoretical basis for this research is a physically based homogenization theory, termed “discrete damage space homogenization method” (DDSHM), which combines micromechanics and thermodynamics to determine the overall response functions of multi-phase materials of arbitrary complexity. The procedure is named DDSHM because the constitutive and evolution equations of the composite are obtained for discrete values of damage (numbers of cracks and crack lengths) and not in terms of an average damage parameter. The micro-crack evolution law used may in general include time and temperature effects as well as other material parameters including changes in constituent and interphase strengths under extended environmental exposures.

In this methodology, a thermodynamically based constitutive relation is formulated using two scalar functions: a thermodynamic potential which specifies the state of the material point; and a dissipation potential which governs the evolution. Given the constitutive relations of the individual phases, both the thermodynamic and dissipation potentials are completely derived by first solving a micromechanics (boundary value) problem, and then performing a homogenization procedure which averages the solution over the chosen RVE. The constitutive and evolution equations (CEE) for the materials to be studied are taken to be functions of a set of internal state variables and a set of damage parameters whose number must be selected based upon some knowledge of the behavior of the micro-structure under load. The derived CEE form a system of ordinary differential equations that describe the evolution of the micro-structure of the RVE. As a result, the FEM based micromechanics analysis can be performed independently of the global structural analysis. The overall approach for deriving the constitutive and evolution equations has already been integrated with the commercial finite element code ABAQUS for analysis of layered polymer matrix composites and is extended here for application to CMCs.

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INTRODUCTION

Ceramic matrix composites (CMCs) represent an important enabling technology for advanced aerospace engine components. Significant progress has been made in understanding the behavior of these complex materials in the linear elastic range, and with some simple forms of progressing damage. However, a general physics-based methodology to assess the initial and lifetime response of complex CMC material architectures with evolving damage would provide a step forward in terms of acceptance and implementation of CMCs in aerospace applications.

For the purpose of discussion we assume that the global analysis of the composite structure is to be conducted using the Finite Element Method (FEM). References [1-4] present a homogenization theory and computational strategy that combines micromechanics and thermodynamics to allow determination of the overall response functions of multi-phase materials of arbitrary complexity. In this work, a thermodynamically based constitutive relation is formulated using two scalar functions: a thermodynamic potential that specifies the state of the material point; and a dissipation potential which governs the evolution. Given the constitutive relations of the individual phases, both the thermodynamic and dissipation potentials can be completely derived by first solving a micromechanics problem, and then performing a homogenization procedure which averages the solution over the chosen representative volume element (RVE). Even in the presence of growing damages, the effective constitutive equations need be determined only once and independently of the thermo-mechanical load path that will *later* be imposed during structural analysis calculations. In other words, this work presents a computational strategy for the derivation of constitutive equations for composites with specific growing cracks that are obtained once and that are valid for any load history while maintaining consistency with continuum thermodynamics. The approach has been termed a discrete damage space homogenization method (DDSHM) because the effective constitutive and evolution equations (CEE) of the composite are obtained for discrete values of damage (numbers of cracks and crack lengths) not in terms of an average damage parameter.

The goal of DDSHM is to deliver an efficient computational procedure for the analysis of composite materials with growing cracks that retains some of the benefits of homogenization theory and micromechanics. In particular, a strategy is sought to derive the fracture mechanics based CEE for a given RVE of material. The data for these equations are computed independently from the global calculation, i.e., the detailed RVE problem is not embedded in the global model. The results are valid for any load history and, therefore, the constitutive equations can be used in any global analysis. This allows the nonlinear material model to be integrated into a commercial finite element code for the structural analysis. This has been accomplished using the general purpose structural analysis code ABAQUS, via user-material subroutines (UMAT) [5].

THEORY

In this section of the paper, the theory of the DDSHM is briefly discussed as pertaining to the macroscopic failure of composites. DDSHM is a computational strategy used to solve the constitutive and evolution equations for a linearly elastic composite with evolving micro-cracks. This physically based method stems from the homogenization theory presented in [1-4] and fracture mechanics. In particular, the effective behavior of the composite material is governed by two scalar functions: a thermodynamic potential and a dissipation potential. The thermodynamic potential, namely the Helmholtz free energy H , is a function of the selected macroscopic state variables:

$$H(t) = H(E_{ij}(t), \lambda_1(t), \dots, \lambda_N(t)) \quad (1)$$

where $E_{ij}(t)$ is the small strain tensor and $\lambda_1(t), \dots, \lambda_N(t)$ are N internal state variables (ISVs), and t is time. The actual constitutive equations are given by

$$\Sigma_{ij} = \frac{\partial H}{\partial E_{ij}} \quad \text{and} \quad G_i = -\frac{\partial H}{\partial \lambda_i}, \quad (2)$$

where Σ_{ij} is the macroscopic stress tensor and G_i is the generalized thermodynamic force promoting the growth of the i_{th} ISV. The dissipation potential Ω is a function of the generalized thermodynamic forces G_i :

$$\Omega = \Omega(G_i), i = 1, \dots, N, \quad (3)$$

and the actual evolution equation for the i_{th} ISV is given by

$$\dot{\lambda}_i = \frac{\partial \Omega}{\partial G_i}. \quad (4)$$

Consider a linearly elastic composite with growing micro-cracks, the ISVs can be chosen as the sizes of the N cracks present in the selected representative volume element (RVE); hence, in this case, G_i represents the energy release rate for the i_{th} crack. From the principles of linear elastic fracture mechanics, the dissipation potential can be expressed as the following form:

$$\Omega = \frac{1}{2} \eta_i \langle G_i - G_i^{cr} \rangle^2, i = 1, \dots, N, \quad (5)$$

where η_i and G_i^{cr} are referred to as the crack growth viscosity coefficient and the critical energy release rate for the i_{th} crack, respectively, and $\langle \bullet \rangle$ denotes the positive part operator defined as

$$\langle \phi \rangle = \begin{cases} 0, & \text{if } \phi \leq 0 \\ \phi, & \text{if } \phi > 0 \end{cases}, \phi \in \Re. \quad (6)$$

Moreover, Eq. (5) yields a crack evolution law for the i_{th} crack:

$$\dot{\lambda}_i = \eta_i \langle G_i - G_i^{cr} \rangle. \quad (7)$$

In order to use the above theory, \mathbf{H} must be evaluated for all possible values of the state variables. In general, it is impractical if not impossible to accomplish this task in an exact sense. In the DDHSM, \mathbf{H} is evaluated at a discrete number of values of the ISVs, and interpolation is then carried out to obtain the general function, e.g. Lagrange polynomials. Specifically, for a given crack state, i.e. the values of λ_i at time t , and based on the effective constitutive equation for the composite Eq. (8),

$$\sigma_{pq}(t) = C_{pqrs}(\lambda_1(t), \lambda_2(t), \dots, \lambda_N(t)) E_{rs}(t), \quad (8)$$

\mathbf{H} can be expressed in terms of the effective moduli and macroscopic strain as:

$$H(t) = \frac{1}{2} C_{ijkl}(\lambda_1(t), \lambda_2(t), \dots, \lambda_N(t)) E_{ij}(t) E_{kl}(t) \quad (9)$$

Here, C_{ijkl} is the effective stiffness matrix for the composite, which is evaluated from micromechanics solution for a representative volume element (RVE).

From Eq. (2) and (7), a system of ordinary differential equations that describe the RVE microstructure evolution in terms of the macroscopic applied strain history can be formed; the evolution of the independent state variables at any point in a loading history and the associated overall material properties can then be determined, given the critical energy release rates. In addition, the effective constitutive equations are determined only once and independent of the thermo-mechanical load path; given an arbitrary loading condition, the associated overall material properties can also be determined. It is also noted that the effective constitutive equations need to be evaluated at various stages of crack development; hence, all possible crack paths within the chosen RVE must be anticipated a priori.

MODELING APPROACH

Three basic steps are required for any constitutive modeling approach: (i) a pre-processing phase, where a model for the local material behavior is created; (ii) a solution phase, where the global structural behavior is determined using information on the evolving material state from the constitutive law; and (iii) a post-processing phase, where material state data is stored for review.

The DDSHM can be viewed as a hybrid methodology which combines classical homogenization theory with the principles of global-local analyses to numerically derive effective constitutive equations that are load history independent and can be obtained separately from a specific global analysis. Indeed, this procedure may be viewed as a computationally efficient alternative to traditional global-local approaches for modeling the effective behavior of composite materials with growing cracks. Items 1-3 (noted by boxes) in Figure 1 highlight the differences

between the DDSHM and the global-local approach. Item 1 is a pre-processing step which is required by the DDSHM but not by the global-local method. Note that the fact that this extra step is performed in the preprocessing phase, i.e., decoupled from the global solution of later structural analyses, is perhaps the most unique and desirable aspect of the DDSHM. The parameter nSOL depends on the damage space discretization, i.e., combines the number of possible crack paths as well as the number of points along each path at which the effective elastic moduli are explicitly calculated. As described previously, this step is currently accomplished using a finite element program written especially for performing the DDSHM procedure.

The major computational difference between the two methods occurs during the solution phase (Items 2 and 3). Crack evolution in DDSHM is determined by numerically solving a set of N ordinary differential equations (ODE's) indicated by the Griffith-type crack evolution law. This is currently accomplished using a 4th order Runge-Kutta algorithm with adaptive (time) step size control. In the global-local method, crack evolution is determined by performing a complete micromechanics analysis for each material point in the global analysis. Hence, if an identical RVE is selected for both the DDSHM and a global-local analysis, the comparison of interest is the computational time required for numerical solution of N ODEs versus solving a mDOF set of linear equations, where mDOF represents the number of degrees of freedom (DOF) in the micro-mechanical solution of the RVE problem. Solving a system of N coupled first order differential equations, where in practice N will in general be on the order 10, will always require significantly less time and computational effort than that needed to carry out the finite element analysis of size mDOF, even if the micromechanics finite element analysis can be conducted without user intervention¹. In other words, for practical problems the computational time associated with performing a micromechanics analysis which involves carrying out a solution for a FE model $p \times q \times \text{mDOF}$ times (i.e., for each global load increment) is expected to be so large that it will considerably outweigh the DDSHM requirement of having to solve nSOL problems to first generate the set of N ODEs which is then solved $p \times q$ times. Furthermore, once the CEE are determined by the DDSHM they can be applied to any global analysis problem of interest. That is, the DDSHM computations carried out in the pre-processing phase are not unique to the global analysis to be conducted. Results of a global-local analysis cannot be re-used for any other problem than that explicitly solved.

¹ As reported in the literature, global-local analyses are commonly conducted by literally extracting force or displacement results from a global analysis and manually applying them to a local model to assess failure. However, it is possible to automate the process. In this case the UMAT routine would be a FE program.

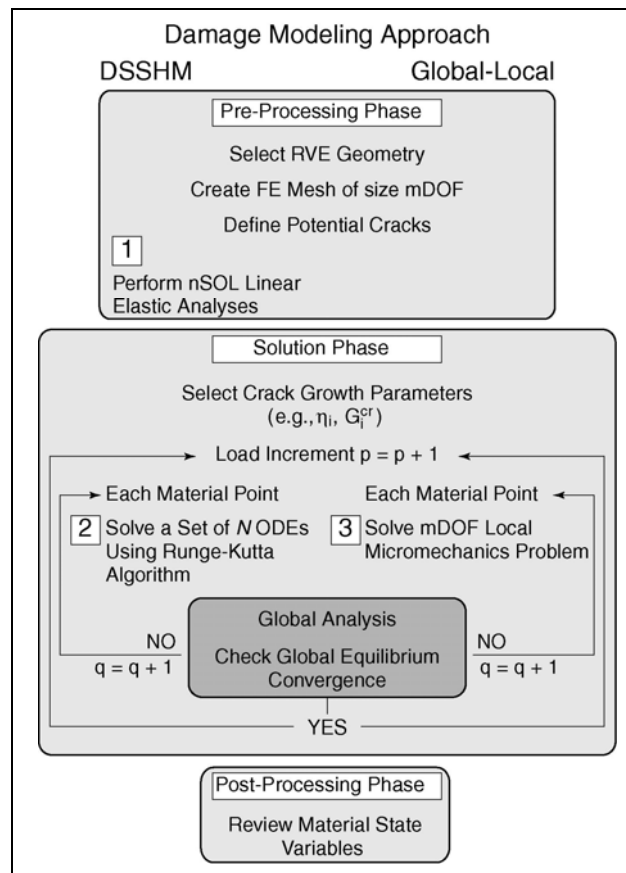


Figure 1. A flow chart showing computational steps for a nonlinear structural analysis. Differences between the DDSHM (left) and a global-local approach (right) are highlighted. The steps shown in the center are common in the two procedures.

The DDSHM approach automatically yields the energy available to grow each possible crack for each material point in the analysis based upon the strain state acting at that point. This is very different than the global-local approach where results of a global stress analysis are reviewed to determine the areas where a local VCCT analysis is to be conducted. If the material properties (G_{cr} and elastic moduli) are assumed to be spatially independent, results using the DDSHM approach immediately indicate where damage onset is expected. The key to the computational efficiency of the DDSHM is the manner in which the available energy release rate G_i is practically computed. The DDSHM derived CEE reduce to a system of ordinary differential equations that describe the RVE microstructure evolution in terms of the macroscopic applied average strain history. Thus, the value of the ISVs at any point in a loading program can be determined through numerical solution of the set of ODEs and not by repeatedly solving a micromechanics BVP for each load state. The DDSHM is general and subject only to those limitations associated with using a RVE approach for determination of effective material properties.

Because the first step in this approach is to build and run a RVE with appropriate material properties and representations of initial crack surfaces, one must determine whether or not the number and location of patches and available

crack paths is sufficiently dense to predict damage evolution in the RVE for all possible load histories. Microstructural data on initial configuration and damage progression in CMCs were examined in order to rationally define cracks paths and identify any CMC characteristics that would have to be incorporated in the code already developed for PMCs. In particular, micrographs for S200-1 which had been selected as the focus for this study [6, 7], indicated that the primary differences were in greater porosity and larger interface/interphase. Images of microcracking and fiber pull-out were similar (c.f. Figure 2) indicating that modeling strategies used previously for GRP might be applied with appropriate modification. In particular, an existing hexagonal array was adapted to include a BN interphase and potential sleeve-like cracks running along the matrix/interphase and fiber/interphase boundaries.

In order to facilitate the creation and meshing of RVEs, Materials Sciences Corp. has developed an add-on for ABAQUS CAE. The add-on was necessary since most FE pre-processors cannot cleanly mesh around internal delaminations. Using this add-on, a delamination may be any open, non-intersecting surface which the user defines by a series of faceted open curves. The add-on lofts straight lines between the vertices of the curves to form the edges of the facets. The add-on then builds a geometric representation of the RVE and assigns mesh seeds to the crack surfaces so that surface nodes will only be placed at the facet vertices. If desired, the user can then intervene and manually use ABAQUS CAE's meshing tools to build the mesh. For example, the user could partition the geometry in order to mesh the RVE with brick elements. Otherwise, the add-on will automatically mesh the RVE with tetrahedron elements. The add-on then inserts double nodes along the delaminations to form free surfaces and saves the mesh and surface information.

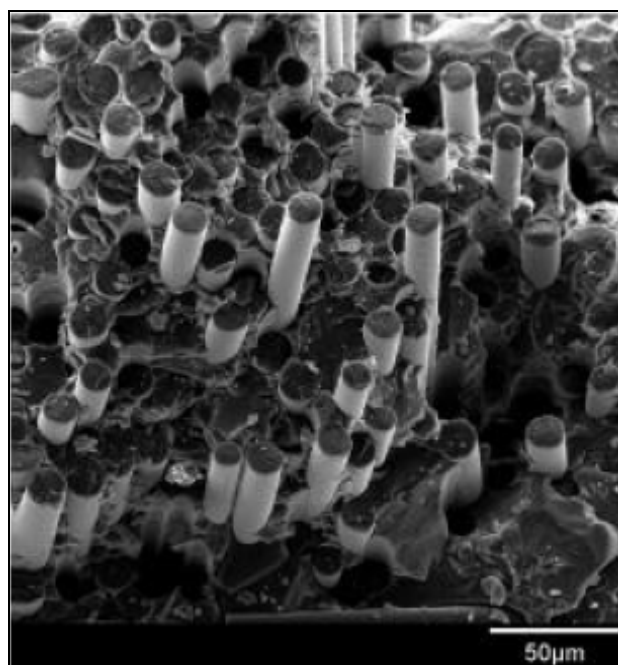


Figure 2. Micrograph of CMC showing fracture surfaces [6].

The input and output files use the XML (Extensible Markup Language) format. The format is supported by the programming languages of the DDSHM project (FORTRAN, Mathematica™, and Python). The format was chosen for its flexibility and shallow learning curve. Prior knowledge of XML is not required to use the software. A Mathematica™ package has also been developed to create the input files.

The resulting hexagonal array RVE included six damage spaces to be implemented in the UMAT: one defining breaks in the fibers, three defining cracks in the matrix, another defining separation between the fiber and the BN coating and lastly a damage space defining the separation between the BN coating and the matrix. Six unique cracks were defined in the RVE. Each crack, or damage space, represents a different mode of failure. Figure 3 details each of the six damage spaces placed in the RVE and the associated damage modes.

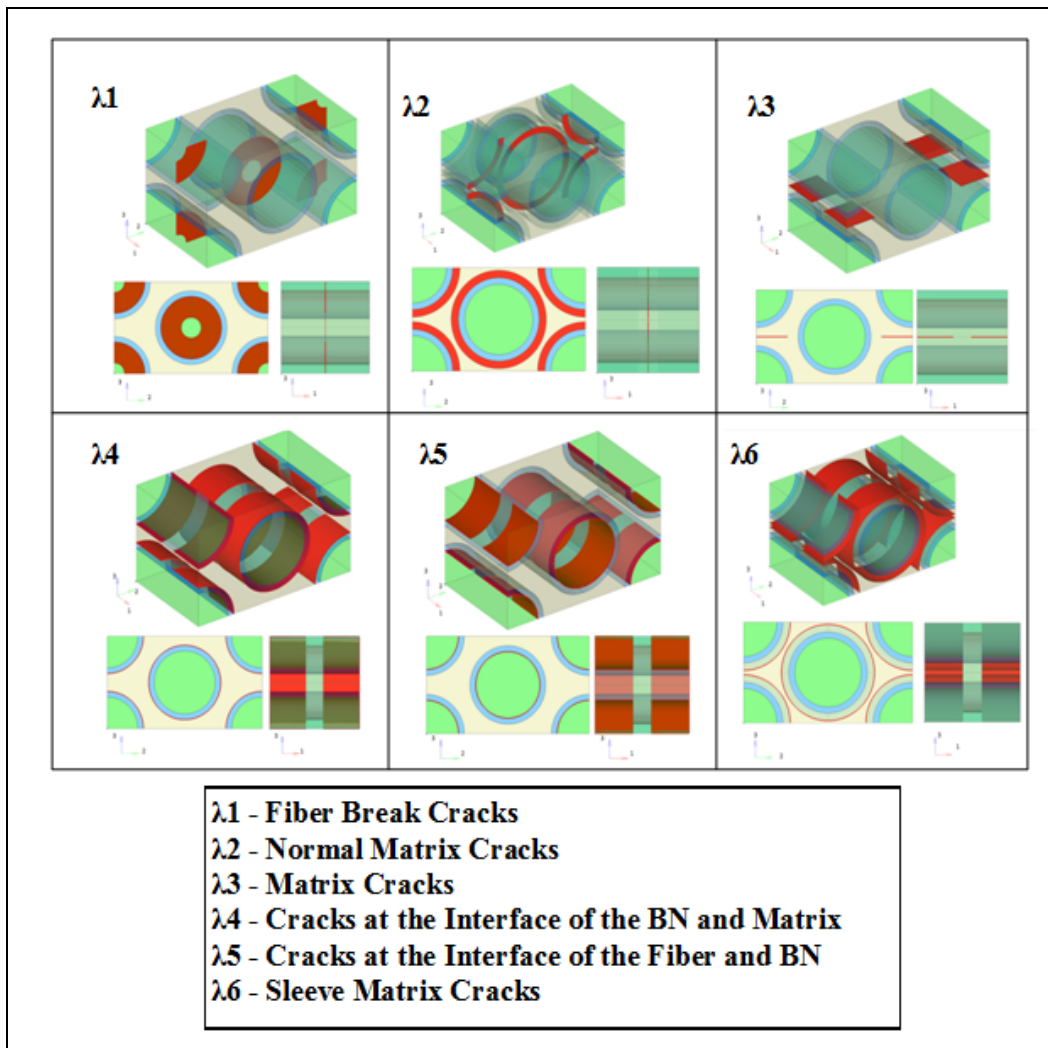


Figure 3. Placed cracks

The resulting UMAT was used along with simple FE model with layered elements oriented to represent a plies in the 0° and 90° directions in order to approximate a woven layer. While a more complex woven RVE could be generated [8], for this initial study the simpler hexagonal array was utilized. To illustrate the functionality of the UMAT, several examples are provided.

First, with reference to Eq. (7), note that η is dependent upon time, where

$$\eta(t) = \frac{\Delta t}{\Delta t_0} \eta_0 \quad (10)$$

where η_0 is the assigned viscosity parameter, Δt_0 is an arbitrary time step and Δt is current time step of the model. This allows the behavior of the damage to be dependent upon on the rate of the applied load and allows for the modeling of creep. Runs with a linearly increasing load for three different values of η , shown in Figure 4, illustrate the effect of this parameter. For smaller values of η , the crack requires more energy to open fully. Larger values of η require less load to open fully and open to the full extend more quickly. Note that for cases shown in the figure, smaller values of η result in slower damage growth and the final damage state is not reached over the range of load analyzed.

Creep tests were also modeled to demonstrate the ability to capture crack growth occurring over time with the loading held constant. Because crack growth due to temperature is an important consideration for CMCs, a model with ends fully-constrained was used to demonstrate crack grow under applied and constant temperature as well (note that for simplicity there is no functional dependence of G_i^{cr} on temperature T). In both cases, the load was ramped for ten load steps and then held for an additional ten steps. Normalized crack growth for the fiber crack is illustrated in Figure 5 and Figure 6 for the mechanical and thermal loads, respectively. In both cases, the crack grows as expected with increasing load or temperature and continues to grow with time as the load or temperature is held.

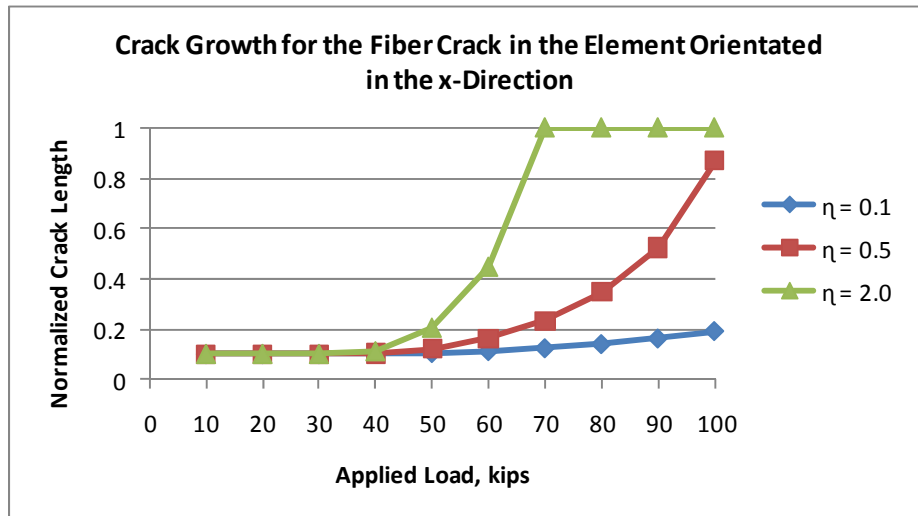


Figure 4. Normalized crack growth for the three values of η

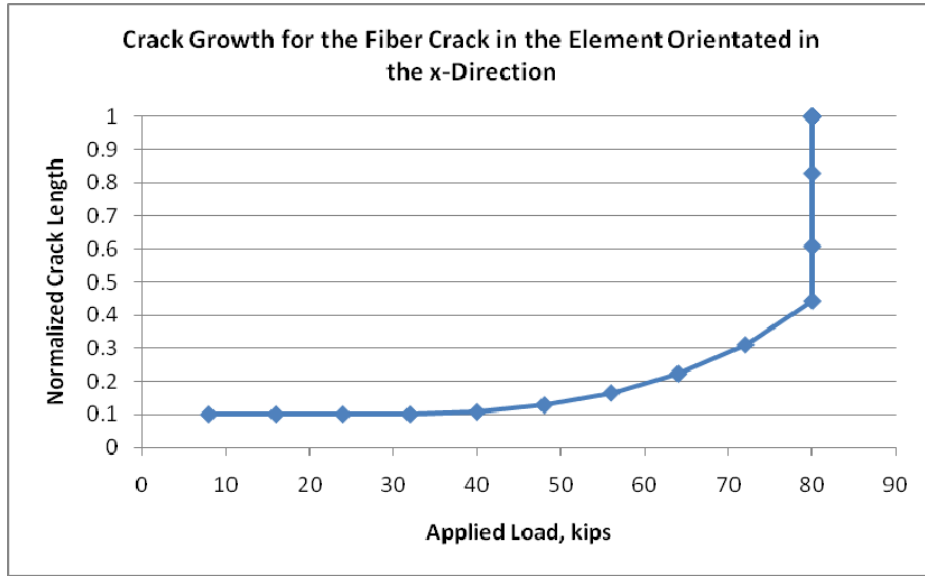


Figure 5. Normalized crack growth for the ramp plus hold load profile

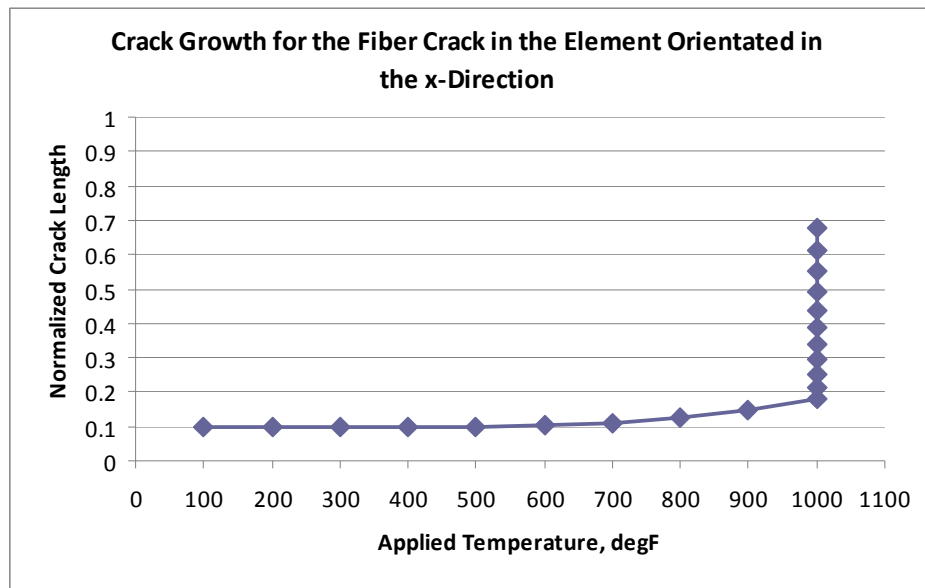


Figure 6. Normalized crack growth for the ramp plus hold thermal profile

An additional analysis, shown in Figure 7, demonstrates the ability to apply loads at different rates and shows the results of applying load at two different rates. The time step, dt , of 1.0 results in an increased rate of the applied load. Thus, the crack opens much sooner and in fewer steps. The time step of 0.1 results in a much slower load rate and crack slowly opens over a number of time steps. The models eventually end at the same damage state but the time it takes each of them is different as is the applied load at which the crack is fully open.

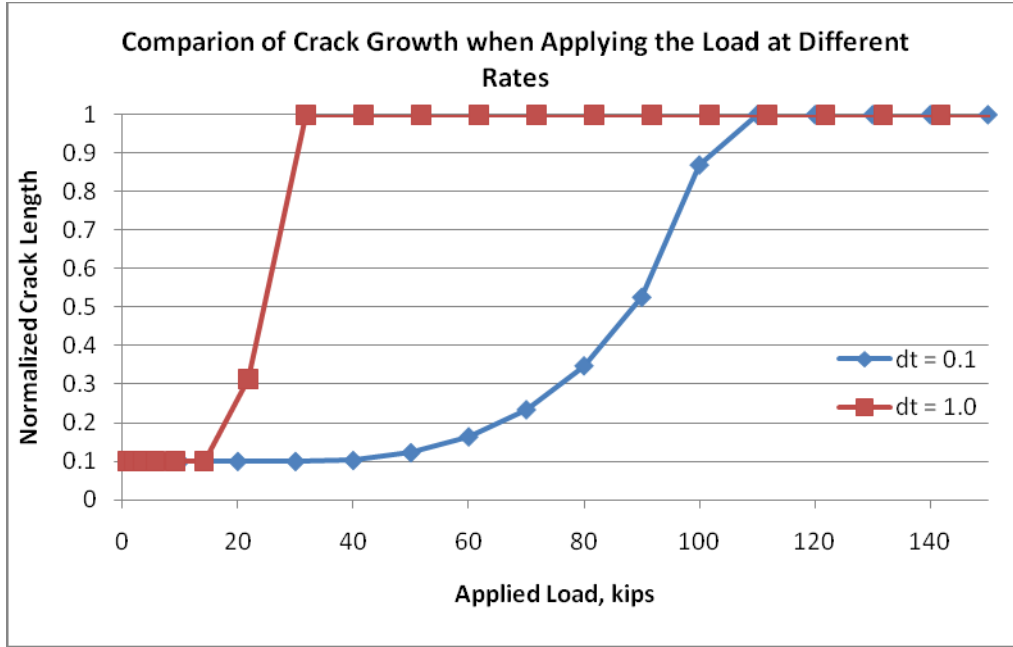


Figure 7. Normalized crack growth at different load rates

RESULTS AND DISCUSSION

This section presents a sample analysis conducted to illustrate the implementation of DDSHM for predicting nonlinear response of ceramic matrix composites. The functionalities demonstrated above allow the modeling of more complex behaviors of materials. However, the focus of the initial study has been on demonstrating integration of the micromechanics model with the commercially available finite element code ABAQUS, via user-material subroutines. Toward that end the UMAT was applied to a simple structural element, a beam in 4-point bending under monotonically increasing load.

Before moving on to presentation of those results, it is important to note that the strain increment to be attempted in each load step is selected by the main ABAQUS program based upon information supplied by UMAT for the previous load increments and thus, is not controlled by the user. The stress increment returned by UMAT is used to check for equilibrium of the structure at the global level (within some numerical tolerance). It is easy to see then that the total computational time in the solution phase shown in Figure 1 depends not only on the number of computations (related to N for DDSHM and $mDOF$ for a global-local approach) performed at the local level but also depends on the stability of the local constitutive routine. Stability here refers to the ability of the local model to return the *expected* updated stress vector and stiffness tensor for the material point to the global model such that global equilibrium is obtained in the fewest iterations possible. An example of an unstable

local model is one where the stiffness and stress residual varies in a discontinuous manner for small values of state variable evolution. Because the effective moduli in the DDSHM are based upon a piece-wise interpolation of values at discrete points of crack evolution, smoothness is achieved through a finite difference technique.

As outlined above, DDSHM approach allows the integration of a nonlinear material model into ABAQUS, a commercial finite element code for the structural analysis. This accomplished by inserting the nonlinear material as a user defined material. Using the RVEs discussed above, ABAQUS FE models were developed for the 4-Point Bending tests shown in Appendix R of [6]. The fracture data available for SiC composites indicates a fairly wide range of SERR values [9, 10]. Therefore the Short Beam Shear data available in the same report was used to determine the values that would result in matrix cracking and/or matrix/interface cracking at the point where nonlinearity becomes apparent in the test data. Another advantage of these UMATs is that layers of elements can be defined with multiple orientations while referencing the same UMAT and the material oriented at ± 45 to represent the woven material in the test specimens.

The UMAT used for these analyses operates by storing the stiffness of an RVE for all possible combinations of crack permutations. As the elements in the finite element model are loaded the UMAT calculates the strain energy release rates (SERRs) for each of the cracks. When the SERR reaches a defined critical SERR for a particular the crack, that crack will begin to open and the stiffness of the element will change in the finite element model to the previously determined stiffness which matches the current state of damage of the element. Thus for the next step of the loading, the stiffness of the damaged elements will have changed, hence, a progressive damage model. The crack opening for each crack type in each element is stored as a state dependent variable and can be plotted in post-processing. This allows the user to view damage progression by crack mode.

The load vs. displacement curve from applying the derived UMAT to the 4-point bending model is compared with experimental data from [6] and the curve for the material with no damage in Figure 8. The comparison with test data is quite good until very close to failure ($P \approx 80$ lb). Driving the model past convergence issues far into progressive failure requires loosening convergence parameters too much to capture the material response however this effect generally provides a reasonable and conservative estimate of ultimate load.

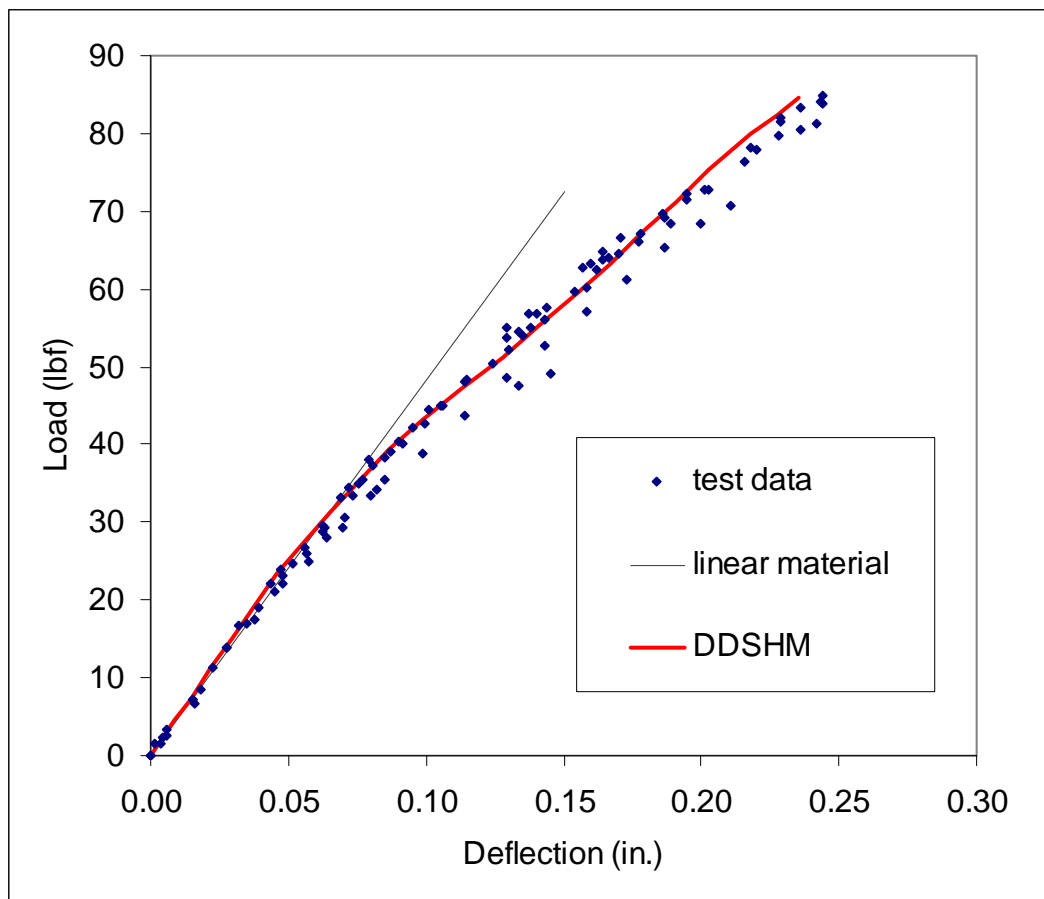


Figure 8. Comparison of 4-pt bend test data for S200-1 [6] with linear material and DDSHM models

Plotting the damage parameters allows features of ceramic matrix composite failure to be examined. For instance, the extent of transverse matrix cracks, matrix sleeve cracks, matrix/interface cracks and fiber cracks are plotted at a point near specimen failure ($P \approx 80$ lb) in Figure 9. Note that as would be expected, transverse matrix cracking is more extensive than anything else and the matrix/interphase cracks have grown over a large portion of the specimen while fiber cracking is far more limited.

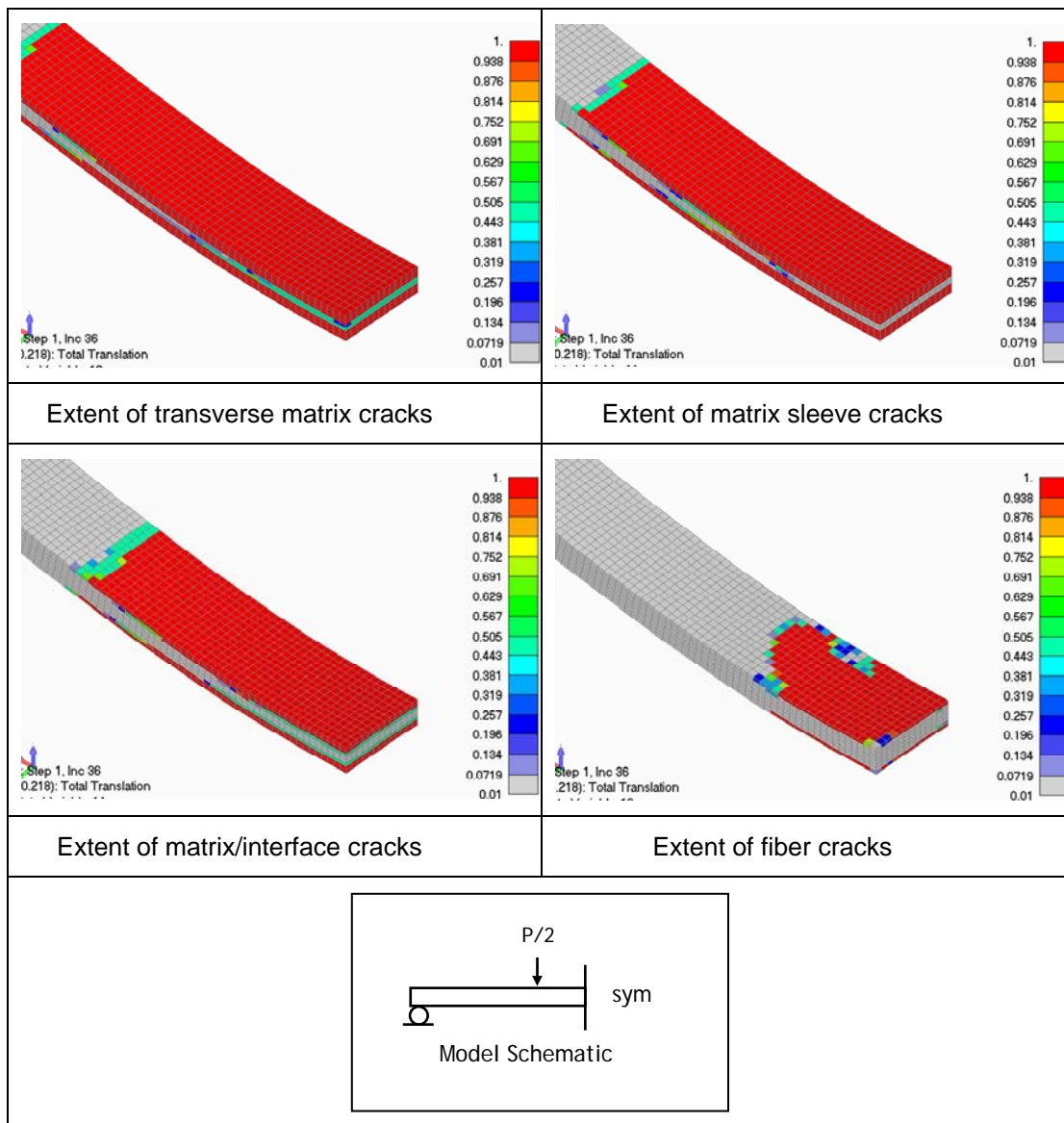


Figure 9. Normalized crack extents at $P \approx 80$ lb for the 4-point bending FEM using the hexagonal array RVE UMAT.

CONCLUSIONS

This paper has presented current work on the development and implementation of representative volume elements to derive the three-dimensional thermo-mechanical constitutive relations for ceramic matrix composites with multiple growing cracks using the discretized damage space homogenization method (DDSHM) approach, which the authors believe represents the most promise for advancing the state of the art in durability modeling. The constitutive and evolution equations developed from the RVE have been integrated and implemented in a general purpose structural analysis code (ABAQUS), via user-material subroutines (UMATs). Simple FE models have been used to demonstrate the code's ability to capture creep,

load rate and thermal effects on damage growth and the method has been further demonstrated using an ABAQUS FE model of a 4-point bending test which has provided good correlation with data from the literature.

While this establishes in principle the usefulness of this approach for the analysis of ceramic matrix composites, further work is necessary. In particular, continuing development will focus on coding the analysis to tie a thermo-oxidation model to the crack evolution law implemented in the RVE.

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